HUB-EP-98/26
MS–TPI–98–6

3D Ising Model with Improved Scaling Behaviour

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Abstract

We present results from the simulation of a two-coupling spin-1 model with states $0, \pm 1$ and nearest neighbour interaction. By a suitable choice of couplings we are able to drastically reduce the effects of corrections to scaling. Our estimates for the critical exponents are $\nu = 0.6299(3)$ and $\eta = 0.0359(10)$. For the universal ratio $Q = \langle m^2 \rangle^2 / \langle m^4 \rangle$ we obtain $Q = 0.6240(2)$. The universal ratio of partition functions with antiperiodic/periodic boundary conditions, respectively, is $Z_a/Z_p = 0.5425(2)$.

1 Introduction

The determination of parameters like critical exponents from finite size scaling [1] is plagued by the appearance of corrections to scaling. Consider, e.g., an Ising model on a cubic lattice of linear extension L. The Binder cumulant

$$Q = \frac{\langle m^2 \rangle^2}{\langle m^4 \rangle} \tag{1}$$

behaves at the critical point like

$$Q(L) = Q^* + q\, L^{-\omega} + \ldots \tag{2}$$

m denotes the magnetization per spin. Q^* is universal. $\omega \approx 0.8$ denotes the leading correction to scaling exponent. Many more terms appear in eq. (2), governed by subleading exponents and combinations of them. If they have non-negligible coefficients in front of them, they can hamper or even make impossible a reliable determination of the infinite L behaviour.

In the language of the renormalization group the presence of strong corrections to scaling is related to the fact that one is far away from the renormalization group fixed point.

In this article, we summarize the results of our attempt to improve the scaling properties of the 3D Ising model by suitably tuning the parameters in a two-coupling spin-1 model that has already been studied by Blöte et al. [2].

We will be mainly interested in the determination of the exponents ν and η that will be obtained from the scaling laws ($i = 1, 2$)

$$\frac{\partial R_i}{\partial \beta} = a_i\, L^{1/\nu} (1 + b_i\, L^{-\omega} + \ldots) \tag{3}$$

and

$$\chi = c + L^{2-\eta} (1 + d\, L^{-\omega} + \ldots)\,. \tag{4}$$

Here, R_2 denotes the cumulant introduced above, and R_1 is the ratio of partition functions Z_a/Z_p, where the subscripts label periodic and antiperiodic boundary conditions, respectively. Antiperiodic boundary conditions are applied in one of the three lattice directions only. The susceptibility χ is defined by

$$\chi = L^3 \langle m^2 \rangle\,. \tag{5}$$

2 Improved Spin-1 Ising Model

Following [2], we consider a spin-1 Ising model on a simple cubic lattice defined through

$$S = -\beta \sum_{<i,j>} s_i \, s_j + D \sum_i s_i^2 \, . \tag{6}$$

The s_i take values $0, \pm 1$, and the spin-spin interaction is a sum over all nearest neighbour pairs. The Boltzmann factor is given by $\exp(-S)$. Blöte et al. chose a fixed $D = \ln 2$, and varied β to tune to criticality. We followed a different procedure, to be described in some detail elsewhere. From prior simulations [3], estimates of the universal quantities R_i^* were available, namely $R_1^* = 0.5425(10)$ and $R_2^* = 0.624(1)$. For a number of lattice sizes L_j ranging from 3 to 14 a sequence of couplings (β_j, D_j) was determined such that $R_i(\beta_j, D_j, L_j) = R_i^*$ within the statistical accuracy. As L increases the pair (β_j, D_j) converges to a point where leading order corrections to scaling vanish. From our numerical results we extrapolate to $(\beta_\infty, D_\infty) = (0.3832, 0.6241)$. We found that this point is approached on the line

$$D \approx -2.04 + 6.95 \, \beta \, . \tag{7}$$

It turns out that eq. (7) is an approximation to the critical line. It is reassuring that the estimate $\beta_c = 0.3934214(8)$, together with $D = \ln 2$ in [2] is close to this line. Our next goal was to approximately identify a second one-dimensional submanyfold of the 2-coupling space, namely that where the leading correction to scaling vanishes. This was possible by fitting the derivatives of the $R_i(\beta_j, D_j, L_j)$ at (β_∞, D_∞) with respect to the two coupling parameters to a certain linear equation. Details will be reported in [3]. Our fit results suggested that the critical line should be approached by varying β while adjusting D according to

$$D = 3 \, (\beta - 0.3832) + 0.6241 \, . \tag{8}$$

A first estimate for β_c was then obtained applying the well established method looking for the crossings of $R_i(L)$ with $R_i(2\,L)$. We used lattices of size $L = 4, 8, 16, 32$ and obtained $\beta_c = 0.383245(10)$, with D given by eq. (8), i.e. $D_c = 0.624235$. This is significantly different from the $D = \ln 2$ used in ref. [2].

3 Simulation Results

Monte Carlo simulations were now performed at $\beta_c = 0.383245$, fixing D according to eq. (8). We simulated on cubic lattices with linear extension L ranging from 4 to 56. State of the art cluster algorithms were employed. Two measurements were separated by three single cluster updates. For the computation of Z_a/Z_p a variant of the boundary flip cluster algorithm [4] was implemented. The runs for the determination of the critical parameters described in the previous section took about 3 months of CPU on Pentium 166-MMX PCs, while the final production runs consumed a total of 1 year.

The data relevant for the present article are summarized in tables 1 and 2. Table 1 gives the quantities R_i, $i = 1, 2$ and χ/L^2. In addition, we quote the number of measurements in the last column. In table 2 we give the estimates of the partial and total derivatives of the R_i with respect to β. Note that eq. (8) implies

$$\frac{dR_i}{d\beta} = \frac{\partial R_i}{\partial \beta} + 3\,\frac{\partial R_i}{\partial D}\,.$$

The quantities in table 2 are multiplied by a factor $f(L) = L^{-1/0.63}$, which compensates to good precision for the leading divergent behaviour with increasing lattice size.

By a reweighting technique we have access also to the same set of observables at a set of four neighbouring β values, ranging from 0.383225 to 0.383265 in steps of 0.000010. Having control over a neighbourhood of the simulation point is important, since we started without a high precision estimate of β_c.

4 Fitting the Data

4.1 Fitting Z_a/Z_p, Q

We first fitted the R_i in order to obtain estimates for the universal quantities R_i^*. The scaling law in question is eq. (2). However, looking carefully at table 1 reveals that corrections to scaling are small. We therefore fitted the data with the law

$$R_i(L, \beta_{MC}) = R_i^* + \frac{dR_i}{d\beta}(L, \beta_{MC})\,\Delta\beta\,. \qquad (9)$$

L	Z_a/Z_p	Q	χ/L^2	stat/10^6
4	.53599(07)	.62408(05)	.87609(13)	30
6	.54080(07)	.62491(06)	.88104(14)	60
8	.54193(09)	.62460(07)	.87706(16)	36
10	.54209(18)	.62464(13)	.87272(33)	10
12	.54248(19)	.62416(14)	.86778(35)	10
14	.54230(21)	.62426(15)	.86399(38)	10
16	.54263(17)	.62409(13)	.86000(32)	13
18	.54251(23)	.62410(17)	.85697(42)	8
20	.54286(28)	.62379(21)	.85332(50)	3
22	.54244(30)	.62404(23)	.85115(55)	7
24	.54229(23)	.62402(17)	.84914(43)	3
28	.54245(31)	.62386(23)	.84373(55)	6
32	.54259(31)	.62390(23)	.84010(56)	6
36	.54213(41)	.62420(30)	.83742(73)	5
40	.54227(32)	.62403(23)	.83392(56)	7
48	.54250(39)	.62395(29)	.82803(69)	5
56	.54272(63)	.62382(47)	.82351(12)	2

Table 1: Results for $R_1 = Z_a/Z_p$, $R_2 = Q$ and the susceptibility divided by L^2 at $\beta = 0.383245$. The last column gives the number of measurements in units of 10^6.

L	$f(L)\,\partial R_1/\partial\beta$	$f(L)\,dR_1/d\beta$	$f(L)\,\partial R_2/\partial\beta$	$f(L)\,dR_2/d\beta$
4	−1.09974(17)	−.63210(11)	.65894(15)	−.09882(03)
6	−1.13595(17)	−.64829(10)	.66236(15)	−.09685(03)
8	−1.14621(20)	−.65290(12)	.66295(18)	−.09614(03)
10	−1.15051(41)	−.65498(24)	.66276(37)	−.09577(07)
12	−1.15293(45)	−.65567(25)	.66307(40)	−.09571(07)
14	−1.15385(49)	−.65661(27)	.66310(46)	−.09555(08)
16	−1.15432(44)	−.65652(25)	.66290(39)	−.09554(07)
18	−1.15547(59)	−.65692(33)	.66294(55)	−.09545(11)
20	−1.15603(71)	−.65732(39)	.66322(64)	−.09553(11)
22	−1.15542(79)	−.65714(43)	.66310(74)	−.09574(17)
24	−1.15675(61)	−.65790(34)	.66419(55)	−.09568(11)
28	−1.15565(80)	−.65730(44)	.66199(75)	−.09520(20)
32	−1.15664(82)	−.65793(46)	.66283(75)	−.09523(18)
36	−1.1568(12)	−.65776(61)	.6638(11)	−.09525(49)
40	−1.15665(84)	−.65785(47)	.66326(84)	−.09557(37)
48	−1.1563(11)	−.65752(59)	.6635(11)	−.09513(58)
56	−1.1562(17)	−.65739(97)	.6628(19)	−.0958(12)

Table 2: Results for partial and total derivatives of $R_1 = Z_a/Z_p$, $R_2 = Q$, multiplied by the factor $f(L) = L^{-1/0.63}$, at $\beta = 0.383245$.

$L_{\min}$	R_1^*	β_c	χ^2/dof
6	0.54143(5)	0.3832516(8)	15.49
8	0.54213(8)	0.3832470(8)	1.78
10	0.54240(10)	0.3832453(9)	0.79
12	0.54251(11)	0.3832447(9)	0.49
16	0.54260(15)	0.3832442(11)	0.46
20	0.54252(25)	0.3832446(14)	0.55
24	0.54226(37)	0.3832457(20)	0.27

Table 3: Fitting R_1 with eq. (9)

$L_{\min}$	R_2^*	β_c	χ^2/dof
6	0.62468(4)	0.3832523(10)	4.59
8	0.62447(6)	0.3832499(10)	2.22
10	0.62429(7)	0.3832479(12)	1.39
12	0.62414(8)	0.3832465(11)	0.42
16	0.62405(12)	0.3832457(14)	0.31
20	0.62393(18)	0.3832447(18)	0.28
24	0.62400(27)	0.3832452(24)	0.23

Table 4: Fitting R_2 with eq. (9)

Here we have included a term which (to first order) corrects for deviations from being at criticality. β_{MC} is our simulation coupling 0.383245, and the $dR_i/d\beta$ are taken from table 2. The fit parameters are R_i^* and β_c entering through $\Delta\beta = \beta_{MC} - \beta_c$. To check for effects from corrections to scaling, the fits were done on a sequence of data sets obtained by discarding data with $L < L_{\min}$. We first fitted separately R_1 and R_2. The results are reported in tables 3 and 4. Then we fitted all data together with three parameters (R_1^*, R_2^*, and β_c). The results are presented in table 5.

Our fit results for Q^* and the β_c's from the Q-fits (as function of $L_{\min}$) are shown in figures 1 and 2. The plots justify our final estimates $R_2^* = 0.6240(2)$ and $\beta_c = 0.383245(1)$. For R_1^* we find 0.5425(2).

$L_{\min}$	R_2^*	R_1^*	β_c	χ^2/dof
6	0.62467(4)	0.54142(4)	0.3832519(5)	10.05
8	0.62441(5)	0.54206(7)	0.3832481(6)	2.19
10	0.62421(6)	0.54231(9)	0.3832463(7)	1.21
12	0.62408(7)	0.54245(11)	0.3832453(8)	0.51
16	0.62399(8)	0.54254(14)	0.3832448(9)	0.42
20	0.62393(13)	0.54252(22)	0.3832446(11)	0.41
24	0.62403(13)	0.54230(22)	0.3832455(11)	0.25

Table 5: Fitting simultaneously R_2 and R_1 with eq. (9)

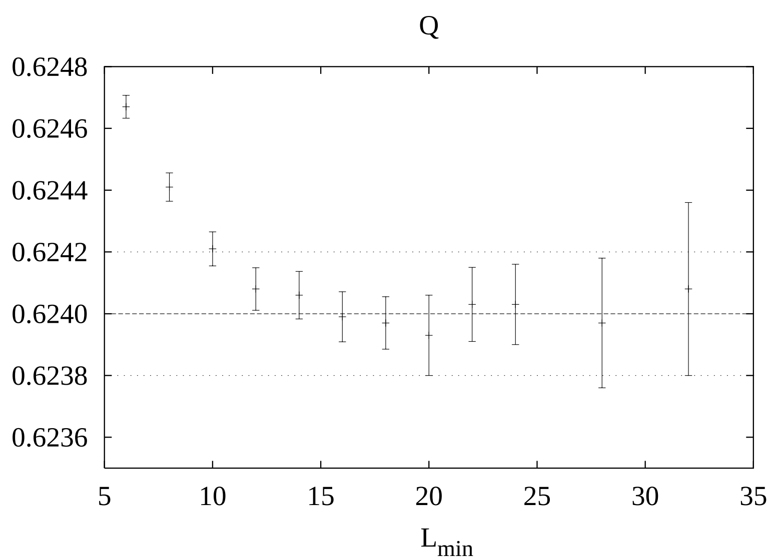

Figure 1: Fit results for R_2^* as function of smallest lattice included in the fit.

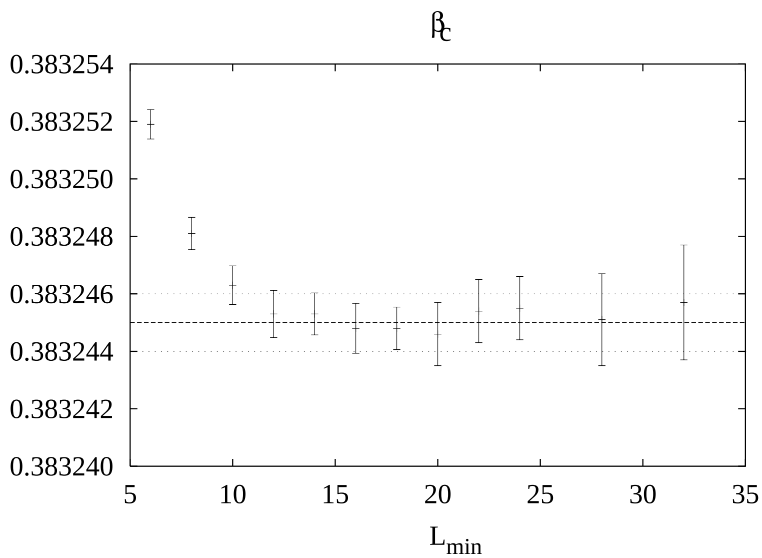

Figure 2: Fit results for β_c as function of smallest lattice included in the fit.

4.2 Fitting the Derivatives of R_i

We fitted our results for the derivatives of the R_i with respect to β, according to the law

$$\frac{\partial R_i}{\partial \beta} = a_i \, L^{1/\nu} \, . \tag{10}$$

Our results for a_2, i.e., for the derivative of the cumulant, are presented in table 6. The ν-results of this table, together with the corresponding results for Z_a/Z_p are plotted in figure 3. Obviously, the derivatives of the cumulant scale much better than those of Z_a/Z_p.

For the derivative of R_1, including the leading correction to scaling *plus* a term $\sim L^{-x}$ with x of order 2 improved the fits. Note, however, that there is more than one exponent or combination of exponents of order 2 (e.g,. $1/\nu+\omega$ or ω'), and fits of this type do not have a sound theoretical basis. The nice scaling behaviour of our data (especially of the cumulant related quantities) allows us to avoid getting into the mess of multi-parameter fits.

To check for the systematic dependence on the location of β_c we repeated the fit for the Q-derivative on data from five shifted β-values from 0.383243 to 0.383247 in steps of 0.000001, covering thus two standard deviations around our β_c estimate. Figure 4 shows that the variation of the ν estimate to this β allows us to put as our final estimate

$$\nu = 0.6299(3). \tag{11}$$

4.3 Fitting the Susceptibility

We fitted the susceptibility data given in table 1, and the corresponding data at shifted β-values with eq. (4). It turned out that the first correction to scaling is negligible. However, the fit results depend to some extent on the location of β_c. The results for the exponent η for $\beta_c = 0.383245$ are given in table 7. Figure 5 shows the η estimates from table 7 and also those from β-values chosen two standard deviations above (upper data) and below (lower data) our β_c estimate.

We then tried to do the fits in an alternative way. Define a function $\beta_c(L)$ by requiring that for any L the relation $Q^*(L, \beta_c(L)) = Q^* = 0.6240$. The susceptibility as a function of L and $\beta_c(L)$ should behave to leading order as

$$\chi \, (L, \beta_c(L)) = \tilde{c} + \tilde{d} \, L^{2-\eta} \, . \tag{12}$$

$L_{\min}$	a_2	ν	χ^2/dof
6	0.66160(42)	0.62969(11)	0.79
8	0.66247(63)	0.62987(14)	0.57
10	0.6622(11)	0.62982(22)	0.60
12	0.6626(12)	0.62989(24)	0.64
14	0.6624(18)	0.62986(36)	0.70
16	0.6622(19)	0.62983(37)	0.77
18	0.6631(23)	0.62998(42)	0.84
20	0.6643(31)	0.63018(56)	0.90
24	0.6662(51)	0.63051(87)	1.18

Table 6: Fitting the derivative of R_2 with respect to β. The fit function is given in eq. (10).

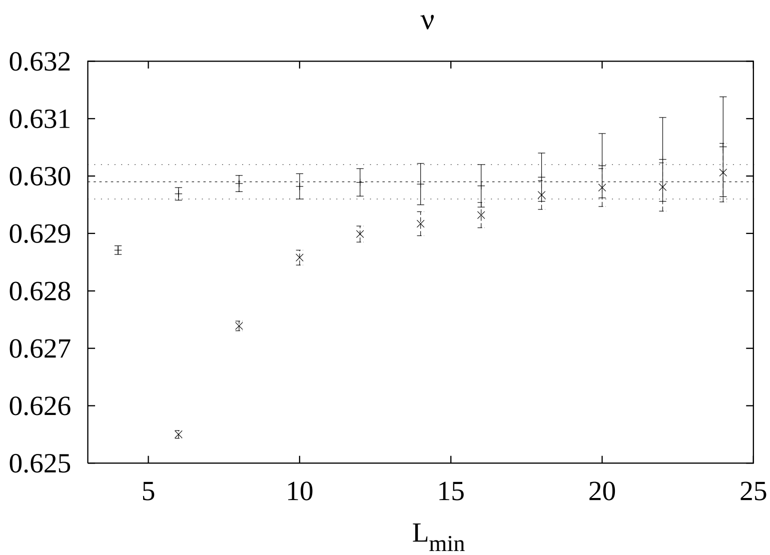

Figure 3: Fit results for ν from fitting $\partial R_i/\partial\beta$ with eq. (10). The data points with the better scaling behaviour belong to the cumulant R_2.

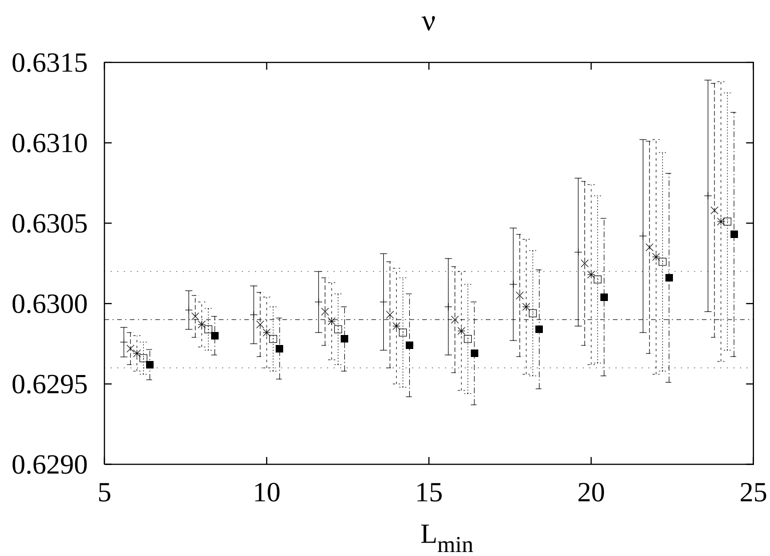

Figure 4: Fit results for ν from fitting $\partial R_2/\partial\beta$ with eq. (10). To check for effects of errors in the location of β_c, the ν-estimate is given for the five β-values 0.383243 to 0.383247 in steps of 0.000001 (left to right).

L_{min}	c	d	η	χ^2/dof
4	–0.5216(56)	0.95751(59)	0.03764(23)	2.30
6	–0.429(17)	0.9526(11)	0.03609(37)	0.51
8	–0.412(47)	0.9520(19)	0.03591(58)	0.54
10	–0.32(11)	0.9501(28)	0.03535(84)	0.49
12	–0.42(17)	0.9517(34)	0.03581(98)	0.50

Table 7: Results from fitting the susceptibilities at $\beta = 0.383245$ to eq. (4).

L_{min}	$\tilde{c}$	$\tilde{d}$	η	χ^2/dof
4	–0.4631(95)	0.9502(10)	0.03528(35)	0.27
6	–0.551(93)	0.9520(24)	0.03580(72)	0.22
8	–0.56(12)	0.9522(26)	0.03587(77)	0.24
10	–0.58(15)	0.9524(31)	0.03594(93)	0.26
12	–0.57(14)	0.9523(29)	0.03589(86)	0.28

Table 8: Fitting the susceptibility at fixed $Q = 0.6240$.

Our fit results are given in table 8 and plotted in figure 6. As a final estimate for η we quote

$$\eta = 0.0359(10)\,. \tag{13}$$

Conclusions

We have demonstrated that the spin-1 Ising model with suitably chosen coupling constants has remarkably improved finite size scaling properties. This allowed us to obtain high precision estimates for the critical indices ν and η and two other universal quantities, the Binder cumulant Q and the ratio of partition functions Z_a/Z_p.

Our results compare very well with a selection of estimates obtained by other authors, quoted in table 9. Many more estimates can be found in refs. [2] and [5]. Our estimate for the cumulant, $Q^* = 0.6240(2)$ may be compared with the one given in [2], namely $Q^* = 0.6233(4)$.

It would be worthwhile to use the present model in studies of physical

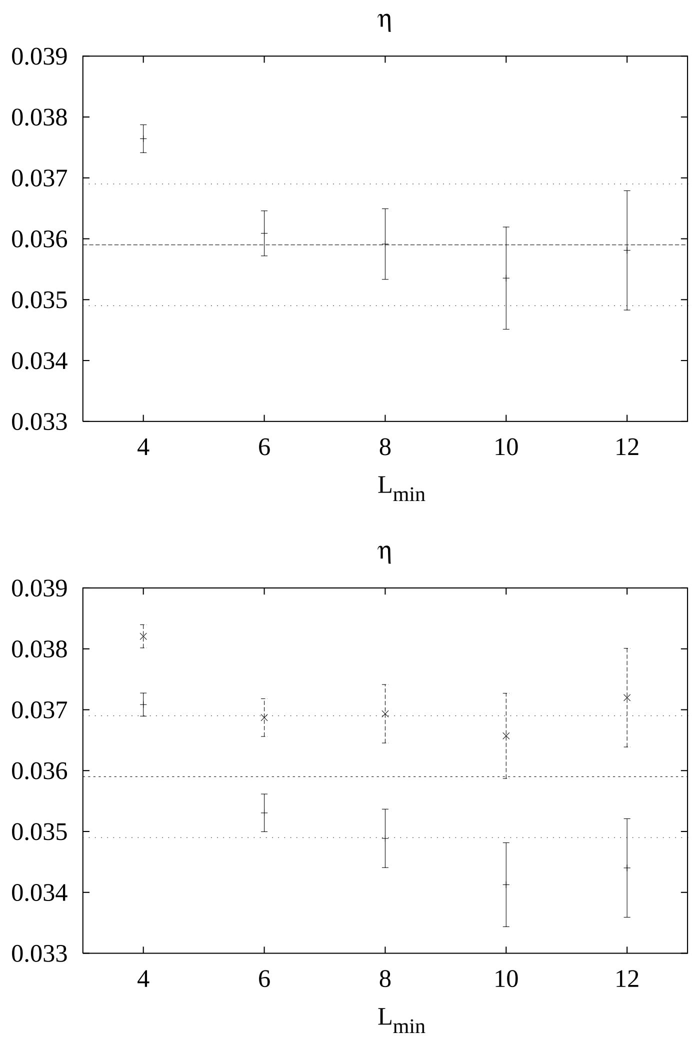

Figure 5: η estimates from fit function eq. (4) as function of $L_{\rm min}$. Top: at our estimated value for $\beta_c = 0.383245$. Bottom: at β chosen two standard deviations above (upper data) and below (lower data) our β_c estimate, i.e. at $\beta = 0.383243$ and $\beta = 0.383247$.

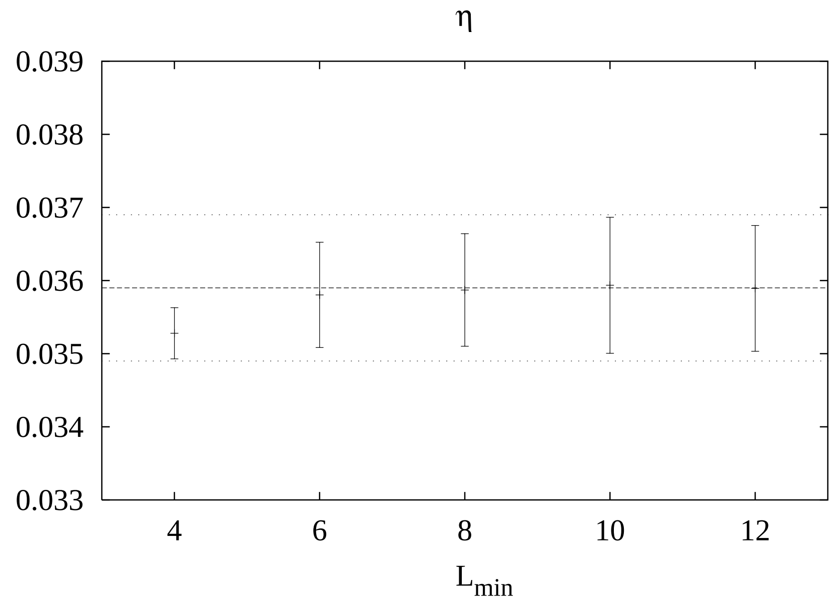

Figure 6: η estimates as function of $L_{\min}$, fitting χ-data at fixed Q to eq. (12).

Ref.	Method	ν	η
[6]	3D FT	0.6301(5)	0.0355(9)
[5]	3D FT	0.6304(13)	0.0335(25)
[5]	EPS	0.6293(26)	0.036(6)
[7]	HT	0.6310(5)	
[2]	MC	0.6301(8)	0.037(3)
[8]	MC	0.6308(10)	
present work	MC	0.6299(3)	0.0359(10)

Table 9: Comparing the results of the present study with previous estimates in the literature. 3D FT means field theoretic calculations directly in three dimensions, EPS refers to ϵ expansion, and MC means that the estimate relies on Monte Carlo simulations.

quantities not discussed in this work and to check to what extent the improved scaling behaviour helps to get better estimates.

Of course, one could also search for even further reduction of corrections to scaling by refining our procedure or choosing variants of the model, e.g., the ϕ^4-model or an Ising model with more couplings. Last but not least, application of the ideas underlying the present analysis to other models seems promising.

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